

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-
59950-41-3 | DTXSID40208664

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.80e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.11e-01

Confidence level: 4.56e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dieldrin</div> <div>Measured: 5.80e-07</div> <div>Predicted: 3.60e-07</div>	<div>Image not found</div> <div>Endrin</div> <div>Measured: 5.80e-07</div> <div>Predicted: 3.60e-07</div>	<div>Image not found</div> <div>Heptachlor epoxide</div> <div>Measured: 5.14e-07</div> <div>Predicted: 3.52e-07</div>
<div>Image not found</div> <div>Kepone</div> <div>Measured: 5.50e-06</div> <div>Predicted: 2.03e-06</div>	<div>Image not found</div> <div>4-Aminoacridine</div> <div>Measured: 6.00e-05</div> <div>Predicted: 1.96e-02</div>	<div>Image not found</div> <div>Nabam-sodium</div> <div>Measured: 7.80e-01</div> <div>Predicted: 2.66e-01</div>